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MICROSCOPIC THEORY OF NON-LINEAR PHENOMENA IN SEMICONDUCTOR SUPERLATTICES

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Publications 1988 - 1989

a. Papers submitted to Refereed Journals and not yet published

J.P.Hagon, M.Jaros and D.C.Herbert, The effect of band structure on Stark shifts in GaAs quantum wells. Phys. Rev. B

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c. Books (and sections thereof) Submitted For Publication

M.Jaros, Microscopic Theory of Ordered Superlattices, to appear in Semiconductors and Semimetals, Guest Editor T.P.Pearsall (At&T)

d. Books (and sections thereof) Published

M.Jaros, L.D.L.Brown and R.J.Turton, Band structure engineering of non-linear response in semiconductor superlattices in Optical Switching in Low Dimensional Systems, p.301 (1989) Plenum Press Eds. G.Haug and K.Balanyi

M.Jaros, Physics and Applications of Semiconductor Microstructures, Oxford Univ. Press, Oxford 1989

g. Invited Presentations at Topical or Scientific Conferences

M. Jaros,
1. Interd. Res. Centre Meeting on DX defects, (U.K.) Imperial College, London, Nov. 1988
2. Annual Solid State Conf. (U.K.) Nottingham , Dec. 1988
3. Electronic Material Conf.(U.S.A.), Boston, June 1989
4. Annual Crystal Growth Conf.(U.K.), Cardiff, Sept. 1989
5. Int. Vacuum and Surface Congress (Germany), Cologne , Sept. 1989
6. Annual Solid State Conf. (U.K.) Warwick, Dec. 1989

h. Contributed Presentations at Topical or Scientific Conferences

NATO workshop on Optical Switching , Marbella, Oct. 1988
Europ. Condensed Matter Conf., Nice, March 1989
Europ. Mater. Res. Soc. Meeting, Strasbourg, May-June 1989
Int. Conf. on II-VI semiconductors, Berlin, Sept. 1989

FINAL REPORT

GENERAL RESEARCH ACTIVITY

In addition to the publication activity reported above I have made a number of presentations and visits associated with this research program. October 88: presented a paper at the NATO workshop on Optical Switching at Marbella, Spain. November 88 : Meeting on Application of Parallel Processing in Band Theory, SERC Daresbury Laboratory, Warrington, U.K., DTI Sponsored Meeting on Advanced Electronic Materials, London, three day visit at RSRE Malvern. In Nov. an invited talk at the Interd. Res. Center Meeting on DX defects (Imperial College). In December I attended the Annual Solid State Conference in Nottingham where I presented an invited paper. March 89: paper at the European Condensed Matter Conf., Nice, France. April: Meeting of the organising committee of the Electronic Materials Conference, Chicago, attended APS meeting at San Louis, and one week visit at IBM Yorktown Heights N.Y. May-June: paper at the European Materials Society Meeting , Strasbourg, France, invited paper at the Boston Electronic Materials Conference, one week visit at IBM, Yorktown Heights , N.Y., one day visit at Fort Monmouth. September: invited paper at the Annual Crystal Growth Conf. Cardiff, U.K., invited paper at the Surface Congress, Cologne, contrib. paper at the Conf. on II-VI Semicond., Berlin, invited paper at the Annual Solid State Conference at Warwick. I had organised a total of 12 days visits by researchers from U.K. and Italy at Newcastle. During this session, I finalised an invited review article on Microscopic Theory of Ordered Superlattices which will appear in Semiconductors and Semimetals as part of a two volume book devoted to strained layer systems, guest editor T.P.Pearsall (AT&T).

SUMMARY OF RESEARCH

The most important conlusions obtained in the course of the work carried out in Newcastle as part of this project are as follows.

1. In our articles published in the Physical Review Letters and in Applied Physics Letters on Si-Ge superlattices, and in the subsequent public polemic inspired by these papers, we have a) refuted the explanation of optical spectra advocated by AT&T Lab (Hybertsen, Lang et al); b) provided the first clear cut argument that shows the importance of defects and interface roughness in interpreting experimental data; this is now an accepted status quo, c) demonstrated the first quantitative study on finite superlattices, with qualitatively new features such new levels, new form of wave functions (e.g. dominance of large wells over small wells in the formation of envelope functions), and localisation at interfaces

2. ~~We have presented~~ a quantitative study of the role of non-ideal interfaces (i.e. those where the two dimensional translational symmetry in the interface plane is not fully preserved). Ours are the first attempt of this kind and our method the only one at present capable of dealing with a problem of this dimension at microscopic level. These studies open the way for realistic studies of interface effects upon transport and optical observables which play a key role in device modelling. This is also the first step towards astablishing a microscopic signature of the interface whicvh one of the outstanding problems in the field of heterostructures.

3. ~~We have~~ demonstarted the possibility to study real geometry structures under strong external fields

4. ~~We have~~ presented a fresh picture of the valley mixing which occurs when states of different bulk momenta cross, for example in GaAs-AlAs structures under hydrostatic pressure or under the influence of a strong external electric field. In particular, we showed that the picture based on particle in a box perturbative models fails to represent correctly even the symmetry related features predicted in our theory and seen in experiments. In particular, we have demonstarted that

this mixing can be used to study the interface quality on the scale of interatomic separation.

We have used our computational scheme to study splitting of the states derived from the secondary X minima and the recombination rates in narrow well GaAs-AlAs superlattices under hydrostatic pressure. We find that in narrow wells the localisation of confined states leads to a breakdown of the second order perturbation mechanism concerning the coupling of bulk states across the Brillouin zone. We have implemented our scheme to provide a detailed picture of the spectra related to the splitting of states derived from secondary valleys in superlattices. These states are a sensitive probe of interface properties.

We have used our method to predict novel structures with infrared transitions in GaAs and Si-Ge microstructures. In particular, we have presented to our collaborators optimised structures in which the infrared transitions can be used as a means of optically characterising these naterials.

We have developed and implemented a computational scheme which enables us to model the electronic structure and electron transitions of quantum well systems in the presence of strong external electric fields without having to resort to approximate treatment. The long term general objective of this effort is to provide a basis for realistic modelling of vertical device structures such as the resonant tunnelling structures, hot electron transistor with a superlattice base, and novel integrated optoelectronic structures. The first stage of this programme has been completed and implemented to study three specific structures. We find that the band structure effect at high fields and in structures with narrow wells and superlattices is quite significant and we have identified its influence on local velocity changes in such structures.

We have modelled the electronic structure of polar interfaces (e.g. GaAs-Ge and showed, in agreement with experiment, that a significant aspect of the present understanding of the formation of localised interface states stems from idealisations used in previous models of such systems.

INTRODUCTION

The interest for a theorist in semiconductor microstructures stems from the possibility of momentum mixing in such structures. This also makes these systems highly "non-linear". Non-linearity is therefore a typical "band structure" effect which cannot be accounted for by simple methods. The manifestations of such momentum mixing we have investigated include coupling of states associated with the principal and secondary minima in the conduction band of GaAs-AlAs, Si-Ge , Ge-Sn, Si-Sn, with and without the presence of external fields, finite structures of certain geometry, interface roughness, coupling of bulk bands due to strain, in narrow wells and barriers, and at indirect interfaces.

In the light of these considerations, we have invested most of our efforts into developing new programmes in such a way that it is possible to include the effect of the breakdown of the translational symmetry both along the growth axis and in the interface plane, and the effect of (weak or strong) electric field, without truncating the description of the electronic structure. Ours is the first effort to account for deviations from strictly periodic order. While a number of efforts have been reported in the literature to account for the effect of an external electric field upon the electronic structure of quantum wells, these studies have been confined to simple tunnelling problems and constrained by the limitations of the transfer matrix technique. This means that either only the simplest structures can be modelled (e.g. a step-like barrier potentials) or that the host band structure must be severely truncated. In essence one has to be able to include in the model a giant block consisting of many hundreds of atoms so that one can not only describe the effect of quantum confinement and electric field upon this microstructure but also retain the signature of the finite nature of the system. This is often difficult to achieve even with techniques based on straightforward wave function matching since one still has to specify the boundary conditions for the incoming and outgoing waves. Our method of calculation is well suited to such requirements since we can deal with very large devices of virtually arbitrary geometry and composition.

MOMENTUM MIXING PHENOMENA

Specific momentum mixing phenomena have been studied in an effort to address topical problems and in the context and as a continuation of complementary projects in Newcastle. A brief summary of some key results highly relevant to the objectives of this project are outlined below. Some of these results have already been published.

We have performed pseudopotential calculations of the nonparabolicity at the conduction band minima of a wide range of GaAs-GaAlAs, GaAs-GaAsP and Si-SiGe superlatices and showed that the position and dispersion of higher lying minbands strongly affect the virtual transitions determining the conduction band nonparabolicity at the band minimum and elsewhere, and the nonlinear response of conduction electrons in general. The role of strain upon the response function was also identified.

We have studied the momentum mixing enhancement of zone-folding effects in type-two superlattices (e.g. Si-Ge, GaAs-AlAs) and showed that the finite nature of the structure (for instance in the five well structures of Si-Ge studied by electroreflectance or in aymmetric GaAs-AlAs MQW and superlattices) and the condition at the interface can alter qualitatively the optical spectra associated with transitions across the gap. Effects such as localisation at interfaces, the effect of external electric field, and changes in transition probabilities across the gap were reported. This has also important implications for modelling existing single and double heterojunction devices where analogous finite element and asymmetry aspects are present. Such effects have so far been excluded from device models based on these structures.

A paper had been compiled by Hagon, Wong and Jaros concerning our study of interface states at polar and strained interfaces and will be published as part of the Proceedings of the Surface Congress at Cologne, Sept. 89 where it will be presented as part of an invited paper. We show that the interface localisation strongly reflects the degree of idealisation in previous models. In particular, for imperfect interfaces we do not expect any significant interface states. Indeed, no such states imlying metallic behaviour have been seen experimentally.

We have studied pressure dependence of cross interface optical spectra in structures studied by Wolford et al at IBM and more recently by Skolnick and coworkers at RSRE. We show that the quadratic perturbation behaviour of the coupling between bulk states across the Brillouin zone changes to quasi-linear when the localisation of the states in the superlatice increases. Although this process may be altered by competing nonradiative recombination effects, our calculation points to the importance of band structure effects in short period superlattices.

In a separate study of momentum mixing in GaAs-AlAs, we have identified new structures where strong optical transitions are expected in the infrared range of wavelenths.

RESULTS FOR QUANTUM STARK EFFECT

At present we can cope with systems whose characteristic dimension is of order 500A. We have tested our scheme on a single and double well/barrier GaAs-GaAlAs system. We find that the quadratic Stark effect in the familiar double barrier structure which has been frequently studied for applications in resonant tunnelling devices actually breaks down at 2×10^{5}V/cm, i.e. much earlier than predicted from simple models. The energy levels of the Stark resonance represented by the peak of the change in the density of states induced by the field, are turning rapidly from the expected quadratic behaviour. On the other hand we show that these effects are not directly due to field induced momentum matrix elements as is commonly believed but that they are structure determined. It is via the structural parameters that the band structure effect of the field must be appreciated. The result has a number of interesting implications not only for transport but also for optical switches operated by excitonic band filling in quantum wells.

A publication on the subject by Hagon, Jaros and Herbert has been accepted in the Physical review B.

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